Khachik Sargsyan

CONTACT INFORMATION

Sandia National Laboratories
Combustion Research Facility
P.O. Box 969, MS 9051
Livermore, CA 94551

Mobile: (734) 730-7454
Work: (925) 294-4885
E-mail: ksargsy@sandia.gov
Web: https://www.ksargsyan.net

Computational scientist with a background in applied mathematics and over 20 years of experience in uncertainty quantification, machine learning, statistical analysis, reduced order modeling and numerical methods, applied to complex computational models in a range of disciplines including climate science, statistical physics, materials science, fluid dynamics.

EDUCATION

University of Michigan, Ann Arbor, MI, USA

- GPA: 4.05/4.00,
- Thesis: "Mean First Passage Times in the Near-Continuum Limit of Birth-Death Processes",
- Ph.D., Applied and Interdisciplinary Mathematics, August, 2007.

Moscow Institute of Physics and Technology, Moscow, Russian Federation

- GPA: 4.86/5.00,
- B.S., Applied Physics and Mathematics, June, 2001.

PROFESSIONAL EXPERIENCE

Sandia National Laboratories, Livermore, CA, USA

- *Distinguished Member of Technical Staff* **2024 - present**
  Leading research projects on uncertainty quantification and scientific machine learning applied to computational models of complex physical phenomena.
- *Principal Member of Technical Staff* **2015 - 2024**
- *Senior Member of Technical Staff* **2010 - 2015**
- *Postdoctoral Fellow* **2007 - 2010**

University of Michigan, Ann Arbor, MI, USA

- *Graduate Student Research Assistant* **2003 - 2006**
  Supported by NSF and Michigan Center for Theoretical Physics. Member of the 3-year NSF research project group "Fronts, Fluctuations and Growth".

Moscow Institute of Physics and Technology, Moscow, Russian Federation

- *Research Assistant* **1999 - 2002**
  Institute for Computer Aided Design of RAS and Institute for System Programming of RAS.

SUMMARY

- Over 70 publications in peer-reviewed journals,
- Over 100 research presentations in academic conferences and workshops,
- Estimated ∼500K lines of scientific programming in Python, C/C++, Matlab, Mathematica,
- Key or lead developer in 4 open-source software products,
- Mentoring over 25 graduate students, postdoctoral fellows and early career researchers,
- Teaching and tutoring of a wide range of undergraduate/graduate level math and engineering classes,
- Bronze medal at the International Math Olympiad in 1997,
- Fluent in English, Russian, Armenian. Reading knowledge of French.

Professional Activities

- Lead PI of SNL LDRD-funded 3-year project "Analysis of Neural Networks as Random Dynamical Systems". Developed state-of-the-art methods for improved training and generalization of neural networks. Demonstrated impact on materials science and climate modeling applications.

- Land Modeling uncertainty quantification lead in DOE BER-funded Energy Exascale Earth System Model (E3SM) project, `e3sm.org`. Developed and deployed automated surrogate modeling and calibration tools for a range of E3SM-based studies, including carbon release, crop modeling, vegetation growth, quasi-biennial oscillation.

- Lead of uncertainty quantification and machine learning components in DOE BES-funded Exascale Catalytic Chemistry (ECC) project, `ecc-project.org`. Developed state-of-the-art methods for combining parametric and intrinsic uncertainties for Kinetic Monte-Carlo models. Developed a new machine learning method, minima-preserving neural network (MPNN), to approximate potential energies in catalytic systems.

- Member of DOE FES-funded FusMatML project. Developed and deployed methods and software for augmenting machine-learned potential energy approximations with uncertainty quantification.

- Member of the DOE FASTMath SciDAC institute, focused on applied math algorithms, tools, and software for HPC applications, `fastmath-scidac.llnl.gov`. Developed state-of-the art methods for model error estimation in physical models. The work has been applied across a range of applications.

- Co-PI of DOE ASCR exploratory project "Uncertainty of Physics-Aware Neural Networtks".

- Current collaboration across multitude of projects with *Brown University, Northeastern University, Emory University, University of Michigan, UCLA, NOAA, LANL, ANL, ORNL, LBLL, PNNL.*

- NNSA ASC, 2020-2021: ASC Artificial Machine Intelligence: developed methods for classification of time series for aging detection.

- SNL LDRD, 2017-2019: Subsystem Reduced-Order Modeling and Network Uncertainty Quantification for Rapid, Agile, Extreme-Scale Simulation. Developed network uncertainty quantification strategies for multi-component systems.

- DOD DARPA, 2016-2018: Uncertainty Quantification in LES Computations of Turbulent Multiphase Combustion in a SCRAMJET Engine. Developed and deployed embedded model error estimation techniques.

- DOE BER-ASCR, 2018-2020: Optimization of Sensor Networks for Improving Climate Model Predictions. Project co-PI. Implemented physics-driven machine learning methods for land model surrogate construction and global sensitivity analysis.

- Participated in the development of Sandia Forecast Model for the COVID-19 Epidemic, 2020: SNL forecasts are used in NM Department of Health to assess the epidemic trends and plan for health resource allocation.

Service

- Editorial Board: Journal of Discrete & Continuous Dynamical Systems – S (DCDS-S) and Journal of Machine Learning for Modeling and Computing (JMLMC).
- Organized several sessions at recognized national and international conferences, such as SIAM UQ, SIAM CSE, SIAM AN, AGU, ISBA, USNCCM, with over 100 speakers total. Co-organized Bay Area Scientific Computing Day Workshop, 2018.
- Invited co-chair at the series of workshops on Artificial Intelligence for Earth System Processes, AI4ESP (`ai4esp.org`): Neural Networks and Surrogate Modeling, 2021.

- Invited participation in the US-Norway bilateral AI forum, 2022.
- Co-chair of Foreign National Networking Group (FNNG) at Sandia, 2020-present.
- Participated or lead over 50 interview panels since 2020. Active participation in WDTS and SULI student intern hiring programs.
- Invited judge for Outstanding Student Participation Award at AGU Fall Meeting 2019.
- Led a SIAM CSE 2023 Affinity Group on Scientific Machine Learning.
- Invited reviewer of multiple proposals to funding agencies: NSF, DOE Office of Science, and Sandia Laboratory Directed Research and Development.
- Invited referee for *Environmental Modelling and Software; Geophysical Research Letters; Scientific Reports; International Journal for Uncertainty Quantification; Computer Methods in Applied Mechanics and Engineering; Structural and Multidisciplinary Optimization; SIAM Journal on Scientific Computing; Journal of Computational Chemistry; International Journal on Chemical Kinetics; SIAM Journal on Uncertainty Quantification; Reliability Engineering and System Safety; Probabilistic Engineering Mechanics; Combustion and Flame; Journal of Computational Science; Mathematics of Climate and Weather Forecasting; Water Resources Research; AIChE Journal; Physics Letters A; Journal of Computational Physics; Journal of Physical Chemistry; Journal of Guidance, Control, and Dynamics; Mathematical Biosciences; AIAA Journal; Multiscale Modeling and Simulation; Physica D; The European Physical Journal B; Computational Geosciences.*
- Member of Society of Industrial and Applied Mathematics (SIAM), American Geophysical Union (AGU), International Society of Bayesian Analysis (ISBA), American Statistical Association (ASA).

Mentorship

- *Postdoctoral (lead advisor):* Nikhil Iyengar (2024-present), Joy Mueller (2022-present), Joshua Hudson (2020-2023), Logan Williams (2022-2023), Varuni Dantanarayana (2020-2021), Vishagan Ratnaswamy (2019-2020), Prashant Rai (2017-2020), Martin Drohmann (2013-2015).
- *Postdoctoral (co-advisor):* Luis Damiano (2023-present), Pieterjan Robbe (2020-2023), Eric Hermes (2018-2022), Xun Huan (2016-2018), Zhen Liu (2012-2014), Thomas Catanach (2017-2018).
- *Sandia Early-Career Mentorship:* Cristian Lacey, Pieterjan Robbe, Moe Khalil, Oscar Diaz-Ibarra, Francesco Rizzi, Tiernan Casey.
- *Graduate Students:* Javier Murgoitio Esandi (2023-present, U of Southern California), Chase Dwelle (2016-2019, U of Michigan, Ph.D. thesis committee member), Katherine Johnston (2020-2022, U of Washington), Haley Rosso (2021-present, Emory U), Sofia Guzzetti (2018, Emory U).
- *Undergraduate Students:* Jonathan Vo (2018-2019, U of California, Irvine), Sarah Teichman (2016, U of Massachusetts), Joseph Heindel (2016, Seattle Pacific Univ.), Cagan Ozen (2016, Columbia U), Jason Bender (2014-2015, U of Minnesota), Chi Feng (2015, MIT).

Software

- Uncertainty Quantification Toolkit (UQTk): a Python/C++ software kit for uncertainty quantification, `sandia.gov/UQToolkit`. Key developer: implemented most of the advanced algorithms present in the library.
- Minima-Preserving Neural Networks (MPNN): a Python library for building neural network approximations to chemistry potentials preserving minima information, `github.com/sandialabs/mpnn`. Sole developer.
- Quantifying Uncertainties in Neural Networks (QUiNN): a Python library centered around various probabilistic wrappers over PyTorch modules in order to provide uncertainty estimation in neural network predictions, `github.com/sandialabs/quinn`. Sole developer.
- FitSNAP: a Python library for building machine learning (ML) potentials based on LAMMPS, `github.com/FitSNAP/FitSNAP`. Developed and implemented uncertainty quantification methods for constructing the ML potentials.

Invited Recent Talks

- "Spatio-Temporal Surrogate Construction and Calibration of E3SM Land Model", ESCO 2024 - 9th European Seminar on Computing, (virtual) Plzen, Czechia, June, 2024.
- "Reduced-Dimensional Neural Network Surrogate Construction and Calibration of the E3SM Land Model", CLM PPE Webinar, virtual, February, 2024.
- "Visualizing and Quantifying Uncertainty of Physics-aware Neural Networks", FASTMath All Hands Meeting, Denver, CO, November 2023.
- "Quantifying Uncertainties in Residual Neural Networks and Neural ODEs", UNCECOMP, 5th International Conference on Uncertainty Quantification in Computational Science and Engineering, Athens, Greece, June, 2023.
- "Climate Model Parameterization with Probabilistic Neural Networks", Bilateral AI US-Norway Forum, Oslo, Norway, October, 2022.
- "Training and Generalization of Residual Neural Networks as Discrete Analogues of Neural ODEs", MLDL Workshop, SNL, July, 2022.
- "Model Error Estimation and Uncertainty Quantification of Machine Learning Interatomic Potentials", Error control in first-principles modelling CECAM-EPFL, Lausanne, Switzerland, June, 2022.
- "Bayesian Inference of Interatomic Potentials: Model Errors and Active Learning", MIT CESMIX-UQ, March, 2022.
- "Active Learning and Uncertainty Quantification for Machine Learning Interatomic Potentials", MMLDT/CSET Mechanistic Machine Learning and Digital Twins for Computational Science, Engineering & Technology, (virtual) San Diego, CA, September, 2021.
- "Quantifying and Reducing Uncertainty in the E3SM Land Model Using Surrogate Modeling", E3SM All Hands Monthly Seminar Series, May, 2021.
- "Probabilistic Methods for Forward and Inverse Uncertainty Quantification", Joint BYU/Utah State Department of Mathematics Seminar, October, 2020.
- "Embedded Model Error Methods", Summer School, Department of Mechanical and Aerospace Engineering University of Rome La Sapienza, September, 2020.
- "Overview of Uncertainty Quantification Methods for Complex Models", DOE Climate Modeling PI meeting, November, 2018.
- "Bayesian Framework for Embedded Model Error Representation and Quantification", Joint Statistical Meetings, Vancouver, Canada, August, 2018.
- "Embedded Model Error Representation for Bayesian Model Calibration", Radcliffe Institute for Advanced Study, Harvard University, May, 2018.
- "Probabilistic Methods for Uncertainty Quantification in Computational Models", MICDE Seminar, University of Michigan, Ann Arbor, April, 2018.

Publications

An up-to-date publication list: `https://scholar.google.com/citations?user=S9st9uEAAAAJ`

[as of 07/17/2024]	All	Since 2019
Citations	2435	1505
h-index	26	21
i10-index	44	31

- F. Ghahari, K. Sargsyan, E. Taciroglu, "Quantification of Modeling Uncertainty in the Rayleigh Damping Model", *Earthquake Engineering & Structural Dynamics*, 53:9, p.2950–2956, 2024.

- K. Blöndal, K. Badger, K. Sargsyan, David H. Bross, B. Ruscic, C. Goldsmith, "Importance Sampling within Configuration Space Integration for Adsorbate Thermophysical Properties: A Case Study for CH3/Ni(111)", *Phys. Chem. Chem. Phys.*, 26, p.17265–17273, 2024.
- L. Williams, K. Sargsyan, A. Rohskopf, Habib N. Najm, "Active learning for SNAP interatomic potentials via Bayesian predictive uncertainty", *Computational Materials Science*, 242, p.113074, 2024.
- F. Ghahari, K. Sargsyan, G. Parker, D. Swensen, M. Celebi, H. Haddadi, E. Taciroglu, "Performance-Based Earthquake Early Warning for Tall Buildings", *Earthquake Spectra*, 40:2, 2024.
- W. Zhou, L. Zhang, A. Sheshukov, J. Wang, M. Zhu, K. Sargsyan, D. Xu, D. Liu, T. Zhang, V. Mazepa, A. Sokolov, V. Valdayskikh, V. Ivanov, "Ground Heat Flux Reconstruction Using Bayesian Uncertainty Quantification Machinery and Surrogate Modeling", *Journal of Geophysical Research - Earth Surface*, 11, e2023EA003435, 2024.
- J. Hudson, M. D'Elia, H. N. Najm, K. Sargsyan, "Measuring Stiffness in Residual Neural Networks", *RAMSES: Reduced order models; Approximation theory; Machine learning; Surrogates, Emulators and Simulators*, p. 153-170, 2024.
- J. Hudson, M. D'Elia, H. Najm, K. Sargsyan, "The Role of Stiffness in Training and Generalization of ResNets", *Journal of Machine Learning for Modeling and Computing*, 4:2, 2023.
- M. Johnson, M. Gierada, E. Hermes, D. Bross, K. Sargsyan, H. Najm, J. Zádor, "Pynta - An automated workflow for calculation of surface and gas-surface kinetics", Accepted, *Journal of Chemical Information and Modeling*, 63:16, 5153–5168, 2023.
- W. Pringle, Z. Burnett, K. Sargsyan, S. Moghimi, E. Myers, "Efficient Probabilistic Prediction and Uncertainty Quantification of Tropical Cyclone–Driven Storm Tides and Inundation", *Artificial Intelligence for the Earth Systems*, 2, e220040, 2023.
- K. Blöndal, K. Sargsyan, David H. Bross, B. Ruscic, C. Goldsmith, "Configuration Space Integration for Adsorbate Partition Functions: The Effect of Anharmonicity on the Thermophysical Properties of CO–Pt(111) and CH3OH–Cu(111)", *ACS Catalysis*, 13:1, pp.19–32, 2023.
- E. Sinha, Katherine V. Calvin, B. Bond-Lamberty, B. Drewniak, D. Ricciuto, K. Sargsyan, Y. Cheng, C. Bernacchi, C. Moore, "Modeling Perennial Bioenergy Crops in the E3SM Land Model (ELMv2)", *Journal of Advances in Modeling Earth Systems*, 15:1, p.e2022MS003171, 2023.
- J. N. Mueller, K. Sargsyan, H. N. Najm, "Polynomial Chaos Surrogate Construction for Stochastic Models with Parametric Uncertainty", *ICASP14: Proceedings of the 14th International Conference on Application of Statistics and Probability in Civil Engineering*, 2023.
- A. Rohskopf, C. Sievers, N. Lubbers, M. A. Cusentino, J. Goff, J. Janssen, M. McCarthy, D. Montes de Oca Zapiain, S. Nikolov, K. Sargsyan, E. Sikorski, L. Williams, D. Sema, A. P. Thompson, M. A. Wood, "FitSNAP: Atomistic machine learning in LAMMPS", *Journal of Open Source Software*, 8(84), 5118, 2023.
- P. Robbe, S. Blondel, T. Casey, A. Lasa, K. Sargsyan, B. Wirth, H. Najm, "Global sensitivity analysis of a coupled multiphysics model to predict surface evolution in fusion plasma–surface interactions", *Computational Materials Science*, 226, 112229, 2023.
- P. Robbe, D. Andersson, L. Bonnet, T. Casey, M. Cooper, C,Matthews, K. Sargsyan, H. Najm, "Bayesian calibration with summary statistics for the prediction of xenon diffusion in UO2 nuclear fuel", *Computational Materials Science*, 225, 112184, 2023.
- E. Hermes, K. Sargsyan, H. N. Najm, J. Zádor, "Sella, an Open-Source Automation-Friendly Molecular Saddle Point Optimizer", *Journal of Chemical Theory and Computation*, 18:11, pp.6974–6988, 2022.
- F. Ghahari, K. Sargsyan, M. Çelebi, E. Taciroglu, "Quantifying modeling uncertainty in simplified beam models for building response prediction", *Structural Control and Health Monitoring*, 29:11, p.e3078, 2022.
- D. Xu, G. Bisht, K. Sargsyan, C. Liao, L. R. Leung, "Using a surrogate-assisted Bayesian framework to calibrate the runoff-generation scheme in the Energy Exascale Earth System Model (E3SM) v1", *Geoscientific Model Development*, 15:12, pp.5021–5043, 2022.

- T.R. Younkin, K. Sargsyan, T. Casey, H.N. Najm, J.M. Canik, D.L. Green, R.P. Doerner, D. Nishijima, M. Baldwin, J. Drobny, D. Curreli, B.D. Wirth, "Quantification of the effect of uncertainty on impurity migration in PISCES-A simulated with GITR", *Nuclear Fusion*, 62:5, p.056007, 2022.
- K. Blöndal, K. Sargsyan, D. Bross, B. Ruscic, C. Goldsmith, "Adsorbate Partition Functions via Phase Space Integration: Quantifying the Effect of Translational Anharmonicity on Thermodynamic Properties", *Journal of Physical Chemistry C*, 125:37, pp.20249–20260, 2021.
- V. Y. Ivanov, D. Xu, M. Dwelle, K. Sargsyan, D. B. Wright, N. Katopodes, J. Kim, V. Tran, A. Warnock, S. Fatichi, P. Burlando, E. Caporali, P. Restrepo, B. F. Sanders, M. M. Chaney, A. M. B. Nunes, F. Nardi, E. R. Vivoni, E. Istanbulluoglu, G. Bisht, R. L. Bras, "Breaking Down the Computational Barriers to Real-Time Urban Flood Forecasting", *Geophysical Research Letters*, 48:20, p.e2021GL093585, 2021.
- B. Kreitz, K. Sargsyan, K. Blöndal, E. J. Mazeau, R. H. West, G. D. Wehinger, T. Turek, C. Goldsmith, "Quantifying the Impact of Parametric Uncertainty on Automatic Mechanism Generation for CO2 Hydrogenation on Ni(111)", *JACS Au*, 1:10, pp.1656–1673, 2021.
- E. D. Hermes, K. Sargsyan, H. N. Najm, J. Zádor, "Geometry optimization speedup through a geodesic approach to internal coordinates", *The Journal of Chemical Physics*, 155:9, p.094105, 2021.
- C. Safta, J. Ray, K. Sargsyan, "Characterization of partially observed epidemics through Bayesian inference: application to COVID-19", *Computational Mechanics*, 66:5, pp.1109–1129, october, 2020.
- V. N. Tran, M. S. Dwelle, K. Sargsyan, V. Ivanov, J. Kim, "A novel modeling framework to secure efficiency and accuracy in real-time ensemble flood forecasting", *Water Resources Research*, 56:3, p. e2019WR025727, 2020.
- E. Hermes, K. Sargsyan, H. N. Najm, J. Zador, "Accelerated Saddle Point Refinement through Full Exploitation of Partial Hessian Diagonalization", *Journal of Chemical Theory and Computation*, 15:11, pp.6536–6549, 2019.
- M. C. Dwelle, J. Kim, K. Sargsyan, V. Ivanov, "Streamflow, stomata, and soil pits: sources of inference for complex models with fast, robust uncertainty quantification", *Advances in Water Resources*, 125, pp.13–31, 2019.
- P. Rai, K. Sargsyan, H. Najm, S. Hirata, "Sparse Low Rank Approximation of Potential Energy Surfaces with Applications in Estimation of AnharmonicZero Point Energies and Frequencies", *Journal of Mathematical Chemistry*, 57, pp.1732–1754, 2019.
- P. P. Tsilifis, X. Huan, C. Safta, K. Sargsyan, G. Lacaze, J. C. Oefelein, H. N. Najm, R.G. Ghanem, "Compressive sensing adaptation for polynomial chaos expansions", *Journal of Computational Physics*, 380, pp.29–47, 2019.
- K. Sargsyan, X. Huan, H. N. Najm. "Embedded Model Error Representation for Bayesian Model Calibration", *International Journal of Uncertainty Quantification*, 9:4, pp. 365–394, 2019.
- D. Ricciuto, K. Sargsyan, P. Thornton, "The Impact of Parametric Uncertainties on Biogeochemistry in the E3SM Land Model", *Journal of Advances in Modeling Earth Systems*, 10:2, pp.297–319, 2018.
- F. Rizzi, K. Morris, K. Sargsyan, P. Mycek, C. Safta, O. Le Maître, O.M. Knio, B.J. Debusschere, "Exploring the interplay of resilience and energy consumption for a task-based partial differential equations preconditioner", *Parallel Computing*, 73, p.16–27, 2018.
- O. Cekmer, K. Sargsyan, S. Blondel, H. Najm, D. Bernholdt,, B.D. Wirth, "Uncertainty quantification for incident helium flux in plasma-exposed tungsten", *International Journal for Uncertainty Quantification*, 8:5, pp.429–446, 2018.
- P. Rai, K. Sargsyan, H. Najm, "Compressed sparse tensor based quadrature for vibrational quantum mechanics integrals", *Computer Methods in Applied Mechanics and Engineering*, 336, pp.471–484, 2018.
- L. Hakim, G. Lacaze, M. Khalil, K. Sargsyan, H. Najm, J. Oefelein, "Probabilistic parameter estimation in a 2-step chemical kinetics model for n-dodecane jet autoignition", *Combustion Theory and Modeling*, 22:3, pp.446–466, 2018.
- J. Kenny, K. Sargsyan, S. Knight, G. Michelogiannakis, J. Wilke, "The Pitfalls of Provisioning Exascale Networks: A Trace Replay Analysis for Understanding Communication Performance",

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- X. Huan, C. Safta, K. Sargsyan, G. Geraci, M. S. Eldred, Z. P. Vane, G. Lacaze, J. C. Oefelein, Habib N. Najm, "Global Sensitivity Analysis and Estimation of Model Error, toward Uncertainty Quantification in Scramjet Computations", *AIAA Journal*, 56:3, pp.1170–1184, 2018.
- X. Huan, C. Safta, K. Sargsyan, Z. P. Vane, G. Lacaze, J. C. Oefelein, H. N. Najm, "Compressive sensing with cross-validation and stop-sampling for sparse polynomial chaos expansions", *SIAM/ASA Journal of Uncertainty Quantification*, 6:2, pp.907–936, 2018.
- F. Rizzi, K. Morris, K. Sargsyan, P. Mycek, C. Safta, O. Le Maitre, O. Knio, B. Debusschere, "Partial differential equations preconditioner resilient to soft and hard faults", *The International Journal of High Performance Computing Applications*, 32:5, pp.658–673, 2018.
- X. Huan, G. Geraci, C. Safta, M.S. Eldred, K. Sargsyan, Z.P. Vane, J.C. Oefelein, H.N. Najm, "Multifidelity Statistical Analysis of Large Eddy Simulations in Scramjet Computations", *AIAA SciTech Forum*, No. AIAA-2018-1180, 2018.
- N. Griffiths, P. Hanson, C. Iversen, A. Malhotra, K. McFarlane, R. Norby, D. Ricciuto, K. Sargsyan, S. Sebestyen, X. Shi, A. Walker, E. Ward, J. Warren, D. Weston, "Temporal and spatial variation in peatland carbon cycling and implications for interpreting responses of an ecosystem-scale warming experiment", *Soil Science Society of America*, 81:6, pp.1668–1688, 2017.
- K. Sargsyan, "Surrogate Models for Uncertainty Propagation and Sensitivity Analysis", "Forward Problems" section, Handbook of Uncertainty Quantification, Springer, 2017.
- B. Debusschere, K. Sargsyan, C. Safta, K. Chowdhary, "The Uncertainty Quantification Toolkit (UQTk)", "Software" section, Handbook of Uncertainty Quantification, 2017.
- P. Mycek, A. Contreras, O. Le Maitre, K. Sargsyan, F. Rizzi, K. Morris, C. Safta, B. Debusschere, O. Knio, "A resilient domain decomposition polynomial chaos solver for uncertain elliptic PDEs", *Computer Physics Communications*, 216, pp.18–34, 2017.
- P. Mycek, F. Rizzi, O. Le Maitre, K. Sargsyan, K. Morris, C. Safta, B. Debusschere, O. Knio, "Discrete A Priori Bounds for the Detection of Corrupted PDE Solutions in Exascale Computations", *SIAM Journal on Scientific Computing*, 39:1, pp.C1–C28, 2017.
- P. Rai, K. Sargsyan, H. Najm, M.R. Hermes, S. Hirata, "Low-rank canonical-tensor decomposition of potential energy surfaces: application to grid-based diagrammatic vibrational Green's function theory", *Molecular Physics*, 115:17-18, pp.2120–2134, 2017.
- M. Khalil, K. Chowdhary, C. Safta, K. Sargsyan, H. N. Najm, "Inference of Reaction Rate Parameters based on Summary Statistics from Experiments", *Proc. Comb. Inst.*, 36:1, pp.699–708, 2017.
- X. Huan, C. Safta, K. Sargsyan, G. Geraci, M. Eldred, Z. Vane, G. Lacaze, J. Oefelein, H. Najm, "Global Sensitivity Analysis and Quantification of Model Error for Large Eddy Simulation in Scramjet Design", *19th AIAA Non-Deterministic Approaches Conference*, No. 2017-1089, 2017.
- K. Morris, F. Rizzi, B. Cook, P. Mycek, O. Le Maitre, O. Knio, K. Sargsyan, K. Dahlgren, B. Debusschere, "Performance scaling variability and energy analysis for a resilient ULFM-based PDE solver", *7th Workshop on Latest Advances in Scalable Algorithms for Large-Scale Systems (ScalA)*, pp.41–48, 2016.
- C. Safta, M. Blaylock, J. Templeton, S. Domino, K. Sargsyan, H. Najm, "Uncertainty Quantification in LES of Channel Flow", *International Journal for Numerical Methods in Fluids*, 83, pp.376–401, 2016.
- K. Morris, F. Rizzi, K. Sargsyan, K. Dahlgren, P. Mycek, C. Safta, O. Le Maitre, O. Knio, B. Debusschere, "Scalability of Partial Differential Equations Preconditioner Resilient to Soft and Hard Faults", *Proceedings of High Performance Computing: 31st International Conference, ISC High Performance 2016*, Frankfurt, Germany, p.469–485, June 19-23, 2016.
- F. Rizzi, K. Morris, K. Sargsyan, P. Mycek, C. Safta, B. Debusschere, O. Le Maitre, O. Knio, "ULFM-MPI implementation of a resilient task-based partial differential equations preconditioner", *Proceedings of the ACM Workshop on Fault-Tolerance for HPC at Extreme Scale*, pp.19–26, 2016.
- J. Ray, Z. Hou, M. Huang, K. Sargsyan, L. Swiler, "Bayesian calibration of the Community Land Model using surrogates", *SIAM/ASA Journal on Uncertainty Quantification*, 3:1, pp.199–233, 2015.

- K. Sargsyan, H. N. Najm, R. Ghanem, "On the Statistical Calibration of Physical Models", *International Journal for Chemical Kinetics*, 47:4, pp. 246–276, 2015.
- F. Rizzi, K. Morris, K. Sargsyan, P. Mycek, C. Safta, O. LeMaitre, O. Knio, B. Debusschere, "Partial differential equations preconditioner resilient to soft and hard faults", *2015 IEEE International Conference on Cluster Computing (CLUSTER)*, pp.552–562, 2015.
- C. Safta, D. Ricciuto, K. Sargsyan, B. Debusschere, H.N. Najm, M. Williams, P. Thornton, "Global Sensitivity Analysis, Probabilistic Calibration, and Predictive Assessment for the Data Assimilation Linked Ecosystem Carbon Model", *Geosci. Model Dev.*, 8, pp.1899–1918, 2015.
- K. Sargsyan, F. Rizzi, P. Mycek, C. Safta, K. Morris, H. N. Najm, O. Le Maître, O. Knio, B. Debusschere, "Fault Resilient Domain Decomposition Preconditioner for PDEs", *SIAM Journal on Scientific Computing*, 37:5, pp. 2317–2345, 2015.
- J.D. Jakeman, M.S. Eldred, K. Sargsyan, "Enhancing l1-minimization estimates of polynomial chaos expansions using basis selection", *Journal of Computational Physics*, 289, pp.18–34, 2015.
- C. Safta, K. Sargsyan, B. Debusschere, H. N. Najm, "Hybrid discrete/continuum algorithms for stochastic reaction networks", *Journal of Computational Physics*, 281:0, pp.177–198, 2015.
- C. Safta, K. Sargsyan, H.N. Najm, K. Chowdhary, B. Debusschere, L.P. Swiler, M.S. Eldred, "Probabilistic Methods for Sensitivity Analysis and Calibration of Computer Models in the NASA Challenge Problem", *Journal of Aerospace Information Systems*, 12, pp.219–234, 2015.
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